Temperature **measurement under the convection and segregation in the vibrated bed of powder: A numerical study**

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Abstract In numerically simulated vibrated beds of powder, we measure temperature under convection by the generalized Einstein's relation. The spatial temperature distribution turns out to be quite uniform except for the boundary layers. In addition to this, temperature remains uniform even if segregation occurs. This suggests the possibility that there exists some *thermal equilibrium state* even in a vibrated bed of powder. This finding may lead to a unified view of the dynamic steady state of granular matter.

1
Introduction

Granular matter is characterized by a set of macroscopic particles, e.g., sand, snow fall, sugar, salt and rice. Recently many physicists became interested in the dynamics of granular matter [1], because it shows many striking features. These include convection, segregation, surface waves, and flows. They are hard to understand by the word of physics, although it is relatively easy to reproduce them numerically.

For example, the concept of granular temperature [1] is often used to describe the dynamical state of powder. However, in contrast to rapid granular flow [2], the granular temperature turns out not to be a good measure for dense granular matter. For example, granular temperature in vibrated beds of powder is anisotropic [3], which is not a favorable feature.

On the other hand, Wildman and Huntley [4] have found useful a temperature that is given by the mean squared displacement curves for short times. Although it sounds promising, their definition is valid only when convective flow is negligible.

Recently Makse and Kurchan [5] have numerically found that the temperature defined by Einstein's relation is well defined and is independent of the size of the particles in granular matter. In contrast to that of Wildman and Huntley [4], Makse and Kurchan's definition is valid even if there is a non-negligible flow. Also D'Anna *et al* [6] have found that their

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variant using AC frequency is also well defined. Thus we may expect that transport phenomena of granular particles can give us a more suitable definition of temperature than the conventional granular temperature.

In spite of these successful applications of Einstein's relation to define the temperature in the granular matter, its application is very limited. This is because the conventional Einstein's relation can be defined only in a spatially uniform system. In order to apply Einstein's relation, we need to understand the long time behavior of tagged particles. If the system is not uniform at all, the tagged particle will travel around various places having various temperatures. Thus what we can measure is a spatially averaged temperature, which cannot reflect spatial structure in the system. On the other hand, if the system is uniform, temperature is uniform, too. This means that we can never know if the thermal equilibrium really stands or not from the measurement of temperature by Einstein's relation. However, as demonstrated by Wildman and Huntley [4], it is not always necessary to observe long time behavior in order to derive temperature from the transport phenomena.

In this paper, we have developed a heuristic method to measure temperature by Einstein's relation in the strongly non-uniform system. In §2, following Makse and Kurchan [5], we introduce the temperature using Einstein's relation. In §3, the heuristic approach to define local temperature is presented, and in §4 this definition is further generalized so as to measure temperature in the system under the flow. The numerical results in vibrated beds are shown in §5, and how segregation affects the temperature is investigated in §6. In §7, we have discussed about the validity of our results; §8 contains summary and conclusion.

2
Einstein's relation and temperature

Suppose there is a particle which obeys a random walk. So as to be simple, we restrict its motion to the one dimensional space. If $x(t)$ is the coordinate of the particle at time t, then the diffusion constant D is defined as

$$\langle [x(t) - x(0)]^2 \rangle = 2Dt,$$

where $\langle \cdots \rangle$ means the ensemble average. On the other hand, the mobility μ can be defined as

$$\langle x(t) - x(0) \rangle = \mu f t,$$

where f is the applied force. When combining the above two equations with the Einstein's relation

$$T \equiv \frac{D}{\mu},$$

where T is temperature, we get

$$T = \frac{f}{2} \frac{\langle [x(t) - x(0)]^2 \rangle}{\langle x(t) - x(0) \rangle}.$$

Recently, Makse and Kurchan [5] used this equation as the definition of temperature in granular matter. They have performed three dimensional distinct element method (DEM) for the periodic sheared system consisting of a binary set of both large and small particles. They measured D and μ along the direction perpendicular to the shear and found that the measured temperature is the same for both large and small particles.

More recently, D'Anna *et al* [6] have experimentally found that the fluctuation-dissipation ratio

$$\frac{S(\omega)\omega}{4\chi''(\omega)}$$

can be a well defined temperature for the vibrated bed, where $S(\omega)$ is the noise power spectrum density of the angular frequency ω and χ'' is the imaginary part of the complex susceptibility. Since this can be regarded as the generalization of the temperature introduced by Makse and Kurchan to the frequency dependent one, these kinds of definition of temperature seem to be valid for granular matter.

However, there is a difficulty to apply the above definitions to general cases. This is because it is impossible to measure the spatial dependence of temperature using these definitions. Makse and Kurchan's definition is valid only for the long time limit, and D'Anna *et al*'s procedure is used to measure temperature only when we can regard a whole vibrated bed as a thermal bath. Thus, it is rather difficult to relate temperature to the statistical mechanics, because in the statistical mechanics local temperatures must be defined. The definitions above cannot provide such information.

3
Heuristic definition of local temperature for a one dimensional system

In order to generalize Makse and Kurchan's definitions to measure local temperature, we propose a heuristic procedure. First, we subdivide the whole system into smaller cells. Each cell has an index i. Next, we define the transition probability of a particle from the ith cell to the jth cell $P(j,i)$. Suppose the spacing between cells is ℓ, a random walker must travel the distance of ℓ in order to go from cell i to cell $i+1$. Thus the averaged time t_0 until this arises is obtained as

$$t_0 = \ell^2/2D.$$

The escape probability of a particle from cell i is

$$P_{out}(i) \equiv \sum_{k=\pm 1} P(i+k, i; f = 0) \propto 1/t_0 = 2D/\ell^2.$$

On the other hand, when a drift force f exists,

$$t_0 = \ell/f\mu,$$

then the flow $J(i)$ along the f direction is

$$J(i) \equiv \ell \sum_{k=\pm 1} kP(i+k, i; f \neq 0) \propto \ell/t_0 = f\mu.$$

Thus

$$T_i = \frac{D}{\mu} = \frac{P_{out}(i)\ell^2/2}{J(i)/f} = \frac{f}{2} \frac{P_{out}(i)\ell^2}{J(i)}$$

is the local temperature at cell i. Of course we do not insist that this is rigorous, but only regard it as a heuristic argument. Also, in order to remove the dependency on f we employ the following definition

$$T_i^{\text{eff}} \equiv \lim_{f \to 0} T_i$$

of the effective temperature.

4
The definition of effective temperature in the system with flow

As an example to test the above heuristic definition of the effective temperature, we employ a numerical simulation of a vibrated bed of powder. In the vibrated bed of powder considered here, there are convective motions of particles. Thus $\langle x(t) - x(0) \rangle$ is not zero even if f is equal to 0. Furthermore, the vibrated bed we deal with is a two dimensional system. Therefore we need some additional modification of the previous definition of the effective temperature T_i^{eff}.

First we subdivide the system into $N_1 \times N_2$ cells, where $N_1\ell$ is the horizontal size of system and $N_2\ell$ is the vertical size of the system. Then we denote the cell as (i, j) if the cell is the ith in horizontal direction and the jth in vertical direction. The flow vector at cell (i, j) is defined as

$$\boldsymbol{J}(i, j; f = 0) \equiv \ell \sum_{k=\pm 1} k \begin{pmatrix} P(i+k, i; j; f = 0) \\ P(i; j+k, j; f = 0) \end{pmatrix},$$

where $P(i', i; j)$ is the transition probability from (i, j) to (i', j) and $P(i; j', j)$ is the transition probability from (i, j) to (i, j') (See Fig. 1).
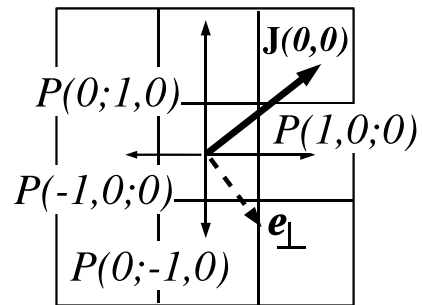

Fig. 1. Schematic figure to explain the relationship among the transition probability P, the flow vector $\boldsymbol{J}$ and the unit vector $\boldsymbol{e}_\perp$ perpendicular to the flow vector. In this example, the center cell is numbered as $(0, 0)$. Thin solid arrows indicate the transition probability, bold solid arrow indicates the flow vector, and broken arrow indicates the unit vector $\boldsymbol{e}_\perp$ perpendicular to the flow vector, along which the force is applied later. The flow vector $\boldsymbol{J}$ of the center cell is $\ell(P(1,0;0) - P(-1,0;0), P(0;1,0) - P(0;-1,0))$. The escape probability of a particle from the center cell $\boldsymbol{P}^{out}$ is $(P(1,0;0) + P(-1,0;0), P(0;1,0) + P(0:-1,0))$.

Next we can define the escape probability of a particle from the cell (i, j) as

$$P_x^{out}(i, j; f = 0) \equiv \sum_{k=\pm 1} P(i + k, i; j; f = 0).$$

Similarly,

$$P_y^{out}(i, j; f = 0) \equiv \sum_{k=\pm 1} P(i; j + k, j; f = 0).$$

In order to deal with vibrated beds, we have to take into consideration the case when $\boldsymbol{J}$ is not zero. We have to find the direction along which the flow is zero when f is equal to zero. Such a direction is perpendicular to the flow vector. Thus the unit vector along this direction is

$$\boldsymbol{e}_\perp(i, j; f = 0) = \frac{1}{|\boldsymbol{J}|} \begin{pmatrix} -J_y(i, j; f = 0) \\ J_x(i, j; f = 0) \end{pmatrix}.$$

The escape probability of a particle from the ith cell along this direction is defined as

$$P_\perp^{out}(i, j; f = 0) \equiv | \, \boldsymbol{e}_\perp(i, j; f = 0) \cdot \boldsymbol{P}^{out}(i, j; f = 0)|,$$

where

$$\boldsymbol{P}^{out}(i, j; f = 0) = \begin{pmatrix} P_x^{out}(i, j; f = 0) \\ P_y^{out}(i, j; f = 0) \end{pmatrix}.$$

Next we apply a small force $f\boldsymbol{e}_\perp$ at cell (i, j). This time, the flow along this axis is defined as

$$J_\perp(i, j; f \neq 0) \equiv \boldsymbol{e}_\perp(i, j; f = 0) \cdot \boldsymbol{J}(i, j; f \neq 0),$$

which takes non-zero values when $f \neq 0$. Using these above, we get

$$T_{ij} = \frac{f}{2} \frac{P_\perp^{out}(i, j; f = 0) \ell^2}{J_\perp(i, j; f \neq 0)},$$

as a local temperature at (i, j). T_{ij}^{eff} is obtained after taking the limit of $f \to 0$ as before.

5
Numerical measurement of the effective granular temperature

The DEM method is the same as in the previous study[7]. The number of particles is 100, the diameter of a particle is 1, and the horizontal size of the vessel is 11. The coefficient of restitution is $e = 0.79$ and $t_c = 0.04$, with $k = 3000$ (spring constant) and $\eta = 6$ (dissipation constant). The strength of interactions with the walls and the bottom is two times larger than the above k and η. The acceleration amplitude $\Gamma = 1.51g$ (g is the gravitational acceleration, here it is taken to be 98, amplitude is 4.11 and angular frequency is 6.20). Figure 2 shows the $\boldsymbol{J}(i, j)$ averaged over sequential 4×10^8 snapshots, where $\ell = 1$. This means $N_x = 11(i = 1, .., 11)$. N_y can be taken as large as possible, but in the present study $j = 1, \ldots, N_y(= 10)$. The $(1, 1)$ cell corresponds to the down-left corner. i and j increases rightwards and upwards, respectively.

As can be seen easily, there is a convective motion over the whole system. The flow pattern is not uniform at all. Also the
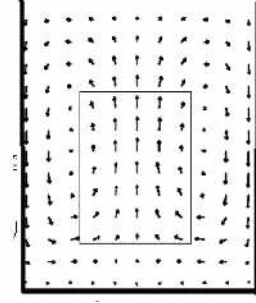

Fig. 2. The flow vectors $\boldsymbol{J}(i, j)$. The flow is upward at the center region and downward at the wall region. The solid rectangle ($4 \leq i \leq 8, 3 \leq j \leq 9$) shows the region where the effective temperature will be computed. The left-bottom corner corresponds to $(i, j) = (1, 1)$ and $i(j)$ increases right(up)wards to $i_{\mathrm{max}} = 11$ and $j_{\mathrm{max}} = 13$.

gravity force is applied. This means that in a naive sense, it is difficult to expect a homogeneous state over the whole system. Thus it will be interesting to see whether thermal equilibrium is kept or not using the above defined effective temperature.

In order to compute T_{ij}^{eff}, first we compute $P(i \pm 1, i; j; f = 0)$ and $P(i; j \pm 1, j; f = 0)$ numerically. Then applying f, we compute $P(i \pm 1, i; j; f \neq 0)$ and $P(i; j \pm 1, j; f \neq 0)$. f should be as small as possible, but too small f cannot generate large enough $J_\perp(i, j; f \neq 0)$ to be estimated. Also if applying f to all the cells at once, global flow structures can be destroyed. Furthermore, we need measurements for several forces before taking $f \to 0$ limit. Considering these requirements, we apply $f/mg = 0.1, 0.2, 0.4, 0.5$ to only a few cells at once (m is the particle mass). Then repeat the same calculation after changing the set of cells to which f is applied. Figure 3 shows the dependence of T_{ij} upon f/mg at cells with $j = 3$. Since they have clear linear dependence upon f, we extrapolate to $f = 0$ using a linear least square fit in order to compute T_{ij}^{eff}. Since the dependence of T_{ij} upon f/mg is similar for other layers, we omit the remaining plots.
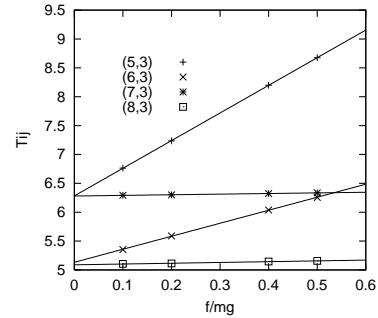

Fig. 3. The dependence of T_{ij} upon f/mg at $j = 3$. Solid lines indicate a linear extrapolation to $f = 0$ using a least square fit. The numbers in parentheses indicate the targeted cells as (i, j).

Figure 4 shows the spatial distribution of T_{ij}^{eff}. We have omitted the regions close to the wall and the bottom ($4 \leq i \leq 8, 3 \leq j \leq 9$). Although T_{ij}^{eff} fluctuates from cell to cell, the

values seem to be close to each other (at least for $i = 5, 6, 7$). Thus surprisingly this suggests the system is more or less in the *thermal equilibrium* state.
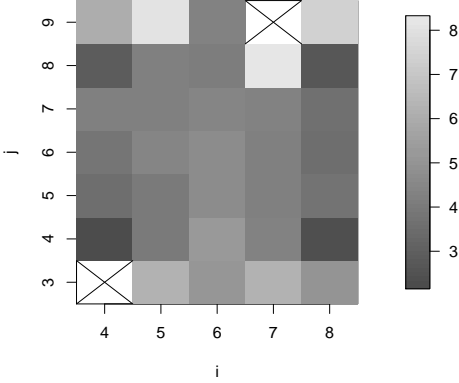

Fig. 4. Spatial distribution of T_{ij}^{eff}. Each row corresponds to a horizontal layer of cells. The whole region corresponds to the rectangle in Fig. 2. Missing values $(i, j) = (4, 3), (7, 9)$ are omitted due to the large error.

In order to confirm this conclusion, we propose the correction equation of T_{ij}^{eff}. Why are these effective temperatures not constant? Does it mean the breakdown of thermal equilibrium? As mentioned above, T_{ij} should be measured along the axis without flow when $f = 0$. For this purpose, we selected the direction perpendicular to the flow direction $\boldsymbol{J}$. However when measuring the effective temperature, a particle can be drifted to the neighboring cells where the flow along drift direction is not zero. In other words, in order that our formulation is satisfied well, the flow in each cell has to be as parallel to each other as it is in Makse and Kurchan's study. Of course, this requirement is not satisfied in the vibrated bed of powder at all.

In order to remove the effect that comes from the fact that the flow vectors are not parallel to each other, we propose here the heuristic equation,

$$T_{ij}^{\text{eff}} = \frac{T_0}{1 + \sqrt{2}} \left(1 + \sum_k \sin(\theta_k - \frac{\pi}{2}) \right),$$

where T_0 is the unperturbed true constant effective temperature, and the summation is taken over the eight neighboring cells, k. θ_k is the angle between the flow vector and the direction of f at cell k (Fig. 5). The supposed meaning of this equation is as follows. $\sin(\theta_k - \frac{\pi}{2})$ is the measure of the flow along f direction relative to neighboring cells. It is proportional to the difference between the neighboring flow vectors if we ignore the difference of absolute values of the vectors as higher order corrections. Thus if it is negative(positive), particles flow in the same(opposite) direction of f. This apparently increases(decreases) the drift caused by f, i.e. the denominator of the definition of the effective temperature, therefore the measured temperature will be smaller (larger) than the true temperature T_0. In order to express this tendency we add $\sin(\theta_k - \frac{\pi}{2})$ to the right hand side. $1 + \sqrt{2}$ is just a numeric

parameter that accounts for the square lattice. The factor 1 represents distance between neighboring cells and $\sqrt{2}$ does that between next neighboring cells. It does not mean anything special at the present study. Figure 6 shows

$$T_0 = \frac{T_{ij}^{\text{eff}}(1 + \sqrt{2})}{\left[1 + \sum_k \sin(\theta_k - \frac{\pi}{2}) \right]}.$$

It takes an almost constant value for all cells. Considering that there are no fitting parameters, our heuristic argument turns out to be very good. Thus we can conclude that the vibrated bed of powder is surely in a thermal equilibrium state.
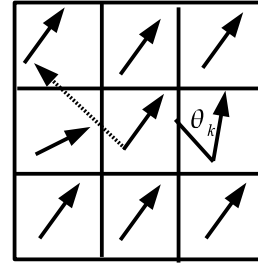

Fig. 5. Schematic figure to show the meaning of the correction equation of the effective temperature T_{ij}^{eff}. Solid arrows indicate the flow vectors at each cell. When we compute the effective temperature at the center cell, we apply a small force f (dotted arrow) to the center cell. However, if the flow vectors at surrounding cells are not parallel to that of the center cell, these accelerate or decelerate the drift caused by f. This occurs when the angle θ_k between the flow vector of surrounding cell and the force direction differs from $\pi/2$.
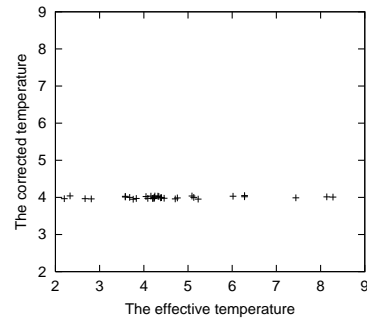

Fig. 6. The corrected temperature as a function of the effective temperature T_{ij}^{eff}. In spite of the large fluctuation of the effective temperature, the corrected temperature takes an almost constant value.

6
Does segregation break the thermal equilibrium?

In the previous section, the effective temperature calculated from the heuristic argument indicates that the vibrated bed of powder is in the thermal equilibrium state. Although the kinetic property, i.e. flow, is non-uniform in the vibrated bed of

powder, particles are the same all over the vessel. Thus it is interesting to see if different particles can also be in the thermal equilibrium state or not. Actually, Makse and Kurchan [5] have shown that particles with distinct sizes have the same effective temperature. However, their system is kinetically uniform.

In this section, we deal with the vibrated bed of powder with different particles. There are many ways to introduce differences among particles. The size difference is the most famous in the vibrated bed of powder, because it causes segregation. However, in our cell approach, different sizes may cause some difficulty because we have employed cells as large as each particle. Different particle size requires different size of cells or another approach.

Let us remind readers that the mixture of glass beads and lead beads causes segregation [8,9]. This phenomenon has already been reproduced by our model [10,11] when we use two kinds of particles with a distinct coefficient of restitution. Thus the segregated state by the introduction of the difference of the coefficient of restitution will provide us the opportunity to see that the thermal equilibrium is satisfied even if the system is spatially non-uniform in both kinetics and material properties. The coefficient of restitution used is $e = 0.67$ ($t_c = 0.04$) [$k = 3200, \eta = 10$] and 0.88 ($t_c = 0.067$) [$k = 1200, \eta = 2$]. The strength of interactions with walls and bottom is two times larger. The acceleration amplitude Γ is taken to be $1.62g$.

From the numerical point of view, a difference from the uniform system occurs only at collisions between different particles. When this occurs, k and η is taken to be the averaged value of these two. Everything else is the same as the previous numerical simulations. Figure 7 shows a snapshot and convective flow patterns. As can be seen easily, two kinds of particles are segregated and convection occurs in each layer independently.

For the calculation of convective flow, we do not distinguish different particles. The effective temperature is measured at each cell as above. Figure 8 shows the dependence of temperature at each cell upon f. Again linearity with f is very good and we get extrapolated values using the least square fits. Fig 9 shows the spatial distribution of temperature. Clearly spatial distribution is much more scattered than that in Fig. 4. This will be because of inhomogeneity of the system. However, applying corrections to this as done in the previous section, we get almost constant values of the effective temperature (Fig. 10), although they are a little more scattered than in the uniform case. Thus it suggests that the thermal equilibrium state is not destroyed even if the system is not uniform. Even when the drastic phenomena like segregation occur, the thermal equilibrium state can still be maintained.

7
Discussion

Although we have found a thermal equilibrium state using the temperature defined by us, there are still some uncertain points in this study. First, the heuristic arguments presented are not substantiated by any first-principles argumentation and the success of the study is judged based on the good uniformity of the effective temperature. Actually our finding that we have obtained a thermal equilibrium state does not always justify our heuristic argument of the temperature. However, even if we cannot justify our results completely, we believe that our findings cannot be accidental. It was very difficulty to find a
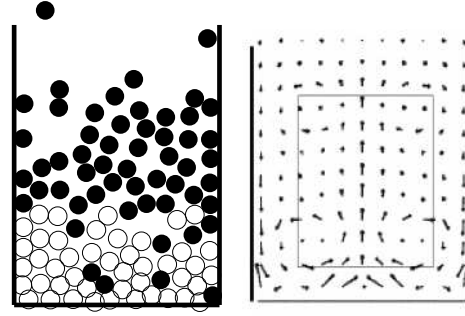

Fig. 7. (a) A snapshot of a segregated bed. Open circles represent particles with the smaller coefficient of restitution. The two kinds of particles are segregated. (b) Flow vectors of the segregated bed. Convective motions are localized at each segregated layer. The solid rectangle shows the region ($3 \leq i \leq 9, 2 \leq j \leq 9$) where the effective temperature will be computed.
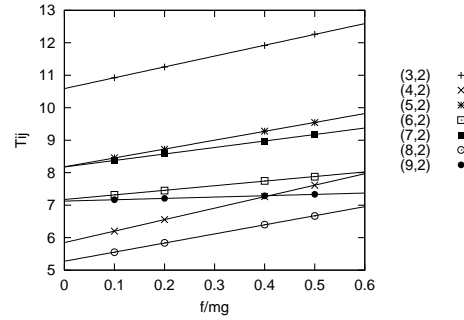

Fig. 8. The dependence of T_{ij} upon f/mg at $j = 2$. Solid lines indicate linear extrapolation to $f = 0$ using the least square fit. The numbers in parentheses indicate the targeted cells as (i, j).

phenomenological temperature definition which characterizes the thermal equilibrium state in the dynamical state of granular matter. Furthermore, our definition is based on the foregoing studies [5,6], thus it has some physical bases although it is not very complete. Our findings can be a start point of understanding general dynamical properties of granular matter.

Second, the numerical model studied here appears to be slightly artificial (two-dimensional, relatively few particles, cells of the same size as the particles, making it impossible to study systems composed of non-monodisperse particles) and therefore the results obtained with this model are not as convincing as they might have been if a different, less restricted model had been employed. The reason why we had to employ such a model is mainly because of the computational limitation. In spite of the apparent easiness of our simulations, it is extremely time consuming. We need very long time simulations in order to suppress the fluctuations. This is because we need the absolute values of fluctuations, not mean values. Compared with getting mean values, measuring fluctuations quantitatively is much more time consuming. Furthermore, we have to repeat numerical simulations because we need extrapolations and the number of points which we can compute at the same time is only a few, as noted above. Of course, it is much more suitable to reproduce these results by more realistic numerical simulations, but it is beyond the scope of this paper. Validating them using more suitable systems will be another future issue.
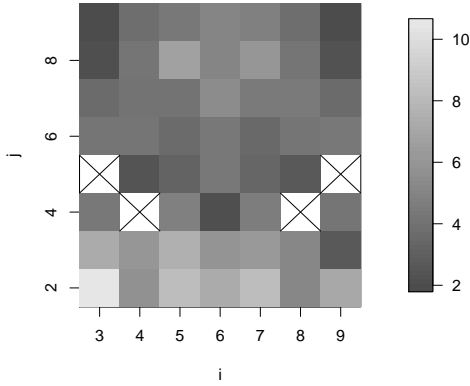
Fig. 9. Spatial distribution of T_{ij}^{eff}. Each row corresponds to each horizontal layer of cells. The whole region corresponds to the rectangular in Fig. 7. Missing values ($(i,j) = (3,5),(4,4),(8,4),(9,5)$) are omitted due to the large error.
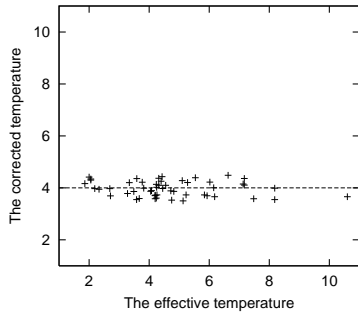

Fig. 10. The corrected temperature as a function of the effective temperature T_{ij}^{eff}. In spite of the large fluctuation of the effective temperature, the corrected temperature takes almost constant value. The horizontal line indicates the mean value of the corrected temperature.

8

Summary and Conclusion

In this study of a granular system, we have introduced heuristic procedures to measure the effective temperature (corrected) proposed by Makse and Kurchan [5]. In the vibrated bed, thermal equilibrium is maintained even if spatial uniformity is kinetically destroyed by convective motion. Also it is still maintained even when segregation occurs in the system. Since the effective temperature is introduced only phenomenologically, it is important to understand this phenomenon by statistical mechanics. However, since clearly energy is not conserved, how to construct statistical mechanics in granular matter is unclear. Although we do not have any clear pictures at the moment, recent findings [12] strongly suggest that statistical mechanics is apparently valid even for the single particle system without collisions. Probably, there is some robustness in the apparent thermal equilibrium system of the dynamics of granular matter.

References

1. H. M. Jaeger, S. R. Nagel and R. P. Behringer, Rev. Mod. Phys. 68 (1996) 1259.
2. I. Goldhirsch, Annual Review of Fluid Mechanics, 35 (2003) 267.
3. R.D. Wildman, J.M. Huntley and J.P. Hansen, Phys. Rev. E 60 (1999) 7066; S. Warr, J.M. Huntley and G.T.H. Jacques, Phys. Rev. E 52 (1995) 5583; R.D. Wildman and J.M. Huntley, Powder Technol. 113 (2000) 14; R.D. Wildman, J.M. Huntley, J.P. Hansen and D.J. Parker, Phys. Rev. E 64 (2001) 051304; R.D. Wildman, J.M. Huntley and D.J. Parker, Phys. Rev. E 63 (2001) 061311; Y.D. Lan and A.D. Rosato, Physics of Fluids, 7 (1995) 1818.
4. R. Wildman and J. M. Huntley, KONA 20 (2002) 105.
5. H. A. Makse and J. Kurchan, Nature 415 (2002) 614; H. A. Makse: Physica A 330 (2003) 83.
6. G. D'Anna, P. Mayor, A. Barrat, V. Loreto and F. Nori, Nature 424 (2003) 909.
7. Y-h. Taguchi, Phys. Rev. Lett. 69 (1992) 1367.
8. Y. Ohyama and I. Uchidate, J. Soc. Powder Tech., Japan 35 (1998) 218 [in Japanese].
9. T. Akiyama, K. Yamamoto and S. Okutsu, Powder Technology 110 (2000) 190.
10. S. Saito, *Numerical Simulation of Inverse Segregation*, Bachelor Thesis, Dept. Phys., Chuo Univ. (1999) [in Japanese].
11. S.Saito, *Numerical Simulation of vibrated bed of powder with two kinds of particles*, Master Thesis, Dept. Phys., Chuo Univ. (2001) [in Japanese].
12. R. P. Ojha, P. A. Lemieux, P. K. Dixon, A. J. Liu and D. J. Durian, Nature 427 (2003) 521.